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METCAN Verification Status

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ABSTRACT

The status of the verification (comparisons of predictions with experimental data) of the METCAN (METal-matrix Composite ANalyzer) code at high temperature is summarized. Verification includes select available room temperature properties of W/Cu composites for different fiber volume ratios. It also includes high temperature comparisons for thermal expansion, moduli, strength and stress/strain behavior for SiC/Ti composites. Furthermore, it includes limited cases for thermal fatigue strength degradation. The verification results summarized, herein, indicate that METCAN simulates complex high temperature metal matrix composite behavior with reasonable accuracy and that it can be used with confidence to identify in-situ nonlinear behavior that influences composite properties.

INTRODUCTION

The nonlinear behavior of high temperature metal matrix composites (HT-MMC) has been investigated at NASA Lewis Research Center during the past decade. The investigation focused on the development of computational simulation procedures and attendant computer codes. One unique aspect of the investigation is that the computational simulation represents the fabrication process which is schematically depicted in figure 1. The investigation culminated in the development of a computer code identified as METCAN (METal-matrix Composite ANalyzer). The simulation capability in METCAN is depicted schematically in figure 2. METCAN has the capability to predict all aspects of HT-MMC behavior, including the fabrication process by using only room temperature properties for the fiber and matrix. The formalism embedded in it, an initial version, and concept demonstration are described in reference 1. A detailed description of the micromechanics to represent the simulation at the constituent materials level is provided in reference 2.

Another unique feature of the computational simulation in METCAN is the introduction of the multifactor interaction model (MFIM) to represent the various nonlinearities and their mutual interactions in the constituents. The equation form of the MFIM and reasons for its selection are summarized in figure 3. A discussion on its ability to represent constituent material behavior and the subsequent influence of this behavior on the response of structural components from HT-MMC is presented in reference 3. METCAN simulation of the cyclic behavior of HT-MMC is described in reference 4, where the influence of the interphase and limited comparisons with room temperature data are also described. METCAN simulation of in-situ behavior and how this can be used to interpret composite measured behavior are described in reference 5.

The cumulative effort invested in the development of METCAN has been substantial, primarily supported by research and technology programs. The support from focused programs (High Temperature Materials, e.g.) is limited to a systematic verification of METCAN including nonlinearities and their mutual interactions. The objective of the present report is to describe the status of this systematic verification of METCAN.

VERIFICATION

The current METCAN verification effort includes: (1) additional room temperature data on tungsten-fiber/copper-matrix (W/Cu) composites for longitudinal tension at three different fiber volume ratios; (2) thermal expansion of SiC/Ti laminates, (3) high temperature strength for a Ti matrix only; (4) high temperature strengths and moduli for SiC/Ti composites, and (5) thermal cyclic loading data (thermal fatigue). Respective values for the room temperature constituent materials properties used as input in the MFIM are summarized in tables I and II. The METCAN simulation begins with the processing and proceeds to cool-down and subsequent loading as is illustrated schematically in figure 4.

Additional Room Temperature Data

METCAN predicted results are compared with W/Cu experimental data (ref. 6). Stress/strain curves in longitudinal tension are shown in figure 5 for a 0.28 FVR composite. METCAN slightly underpredicts the stress/strain curve compared to the experimental data. One reason for this slight underprediction is that the exponent (m) in the stress term in the MFIM (fig. 3) needs a slight adjustment. The adjustment of this exponent consists of arbitrary perturbations until the predicted curve shape matches the measured shape. Similar comparisons are shown in figure 6 for 0.536 FVR and in figure 7 for 0.674 FVR. METCAN consistently underpredicts the experimental data in the middle part which can be remedied by adjusting the stress-term exponent (m) in the MFIM as was already mentioned. In the absence of experimental data the exponents of 0.25 for fiber properties and 0.5 for matrix properties are suggested based on experience to date.

Collectively, the comparisons in figures 5 to 7 lend credence to the use of the MFIM to represent nonlinear stress strain behavior using only room temperature data for fibers and matrix. In addition, METCAN predictions are in good agreement with measured data, especially for composite strengths.

It is worth noting that the in-situ fiber tensile strength for the tungsten fibers in table I is only approximately known. For the comparisons presented in figures 5 to 7, the in-situ tensile strength was estimated using the measured strength for the 0.536 FVR composite. This value was then used to predict the stress/strain curves for the other two composites. This can be used as a guideline for selecting in-situ values for the primitive variables in the MFIM.

Thermal Expansion Coefficients

METCAN predictions for (0/90/0) SiC/Ti laminates are compared with experimental data (ref. 7) in figure 8 for thermal expansion along the 0° ply direction and in figure 9 for thermal expansion along the 90° ply direction. The predictions are almost identical with the data except above 1000 °F for the expansion along the 90° ply direction, where the data indicate a rapid jump. Assuming the data are correct, then, two probable causes may have contributed to this jump. The first is probable interfacial damage in the 90° ply and the second is probable interply layer damage between the 0° plies and the 90° ply. Both of these phenomena are presently being investigated with METCAN by adjusting the properties of the interphase. Data to be generated from the planned experimental program (described later) will further clarify the cause for this rapid jump.

High-Temperature Stress-Strain Behavior

METCAN predicted stress/strain behavior for Ti15 matrix, only (using the default value 0.5) is compared with bulk-matrix measured data in figure 10. The data were obtained at 1022 °F (ref. 8). METCAN overpredicts the stress beyond 0.5 percent strain and the stress at fracture by about 10 percent. The comparison can be improved by adjusting the stress term exponent (m). METCAN predictions for Ti-3Al alloy matrix tensile strength at temperature are compared with data (ref. 9) in figure 11. The comparison is very good except at 800 °F. The data at this temperature are suspect for this discrepancy. These comparisons are considered to be remarkable since nominal, room temperature data available in the databank of METCAN were used in the predictions.

METCAN predictions are compared with measured data (ref. 10) in figure 12 for transverse tensile stress/strain behavior. The composite, the fiber volume ratio, and the temperature are shown in the figure. The comparisons are acceptable considering the relatively large strains to fracture (about 3 percent). The primitive variables for in-situ matrix strength need some readjustment to obtain better comparisons; however that was not done in this investigation. This is consistent with the discussion in the last section for the Ti matrix stress/strain behavior comparisons.

Moduli and Strengths

METCAN predicted longitudinal (11) and transverse (22) moduli (E) for SCS-6/Ti15 at 0.33 FVR are compared with measured data (ref. 11) in figure 13 for two different temperatures. Note that the METCAN predictions are for a composite with no interphase and one with a carbon-rich interphase, with a thickness equal to about 1 percent of the fiber diameter (approximate size from metallographic studies). The predicted values with the interphase are in excellent agreement with the measured data for the transverse modulus while those without interphase are in better agreement with the measured data for the longitudinal modulus. Apparently the interphase contributes significantly to transverse properties and has negligible effect on longitudinal properties.

The comparisons with no interphase are considered to be in good agreement for both moduli at both temperatures. Inclusion of the interphase improves the

comparisons for the transverse modulus while it worsens, somewhat, those for the longitudinal modulus. In either case, the conclusion is that METCAN can be used to predict high temperature moduli with confidence.

Similar comparisons are shown in figure 14 for longitudinal and transverse tensile strengths. For these strengths the METCAN predictions with the interphase are in excellent agreement with the measured data (ref. 11). The comparisons, therefore, indicate: (1) an interphase is likely to develop in SCS-6/Ti composites due to interdiffusion; (2) this interphase must be included in the computational simulation; and (3) METCAN can be used to simulate this complex behavior with the type of data readily available from material suppliers.

Thermal Cycling

Verification for thermal cycling (thermal fatigue) requires reasonably good estimates of the primitive variable N_{TF} in the MFIM. The preferred procedure to estimate this primitive variable is from available composite thermal fatigue data. In the absence of these data, two alternatives are recommended. The first alternative is suitable when the composite has not yet been made but the candidate matrix material is available for which an S/N curve can be generated. Values for N_{TF} and N_{MF} can be estimated from this curve as is shown in figure 15. The second alternative is recommended when composites from the candidate fiber/matrix constituents can be made. This alternative requires the cyclic testing of $[0/90]_s$ composites as is depicted schematically in figure 16. The number of cycles accumulated when the first transply crack develops in the 90° plies is used in the MFIM together with the stress range and temperature range to back calculate N_{TF} and N_{MF} . These values are then used to generate thermal/mechanical fatigue strength, or any other property, degradation curves that can be compared with data for different conditions.

METCAN predicted thermal fatigue degradation effects on longitudinal tensile strength are compared with measured data (ref. 9) in figure 17. For these comparisons N_{TF} was estimated to be about 3000 cycles from the available measured data. The comparisons are excellent in view of the fact that this is a relatively complex thermal cycle. The comparisons further confirm that METCAN has the versatility to accurately simulate the complex nonlinear behavior of high temperature metal matrix composites.

FUTURE PLANS

The future plans for METCAN verification include continuous checking with any high temperature data that become available as well as data from a planned experimental program. The planned experimental program is a grant with Northwestern University. The number of tests and types to be performed are summarized in table III. These specimens were mainly selected to provide sufficient data to verify the MFIM in figure 3. This program has been slow in getting started due to delays in material delivery and delivery of suitable high-temperature specimen grips.

SUMMARY

The METCAN verification status for high temperature metal matrix composites is as follows:

1. Room temperature - satisfactory
2. Thermal expansion - satisfactory
3. Longitudinal and transverse moduli at high temperature - satisfactory
4. Longitudinal and transverse tensile strengths at high temperature - satisfactory
5. Stress-strain curves at high temperatures - adequate
6. Thermal fatigue - satisfactory

CONCLUSION

METCAN successfully simulates the complex behavior of high temperature metal matrix composites. Continuing use and familiarity will enhance its credibility to the point where it can be used with more confidence.

REFERENCES

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TABLE I. - FIBER PROPERTIES FROM METCAN DATABANK

Property	Fiber code names			
	SiC1 ^a	SiC2 ^b	SiC3 ^c	Tung ^d
Df, mils	5.700	5.700	5.700	10.0
Rhof, lb/in. ³	0.108	0.108	0.110	0.683
Tempmf, °F	4500.000	4500.000	4870.000	6170.0
Ef11, Mpsi	50.700	50.800	60.000	59.0
Ef22, Mpsi	50.700	50.800	60.000	59.0
Nuf12, in./in.	0.190	0.250	0.300	0.29
Nuf23, in./in.	0.190	0.250	0.300	0.29
Gf12, Mpsi	21.300	20.300	23.100	22.7
Gf23, Mpsi	21.300	20.300	23.100	22.7
Alfaf11, ppm/°F	1.200	2.720	2.700	2.5
Alfaf22, ppm/°F	1.200	2.720	2.700	2.5
Kf11, Btu/hr/in./°F	0.806	0.806	0.806	8.28
Kf22, Btu/hr/in./°F	0.806	0.806	0.806	8.28
Cf, Btu/lb	0.300	0.300	0.300	0.024
Sf11T, ksi	486.000	500.000	500.000	350.0
Sf11C, ksi	486.000	500.000	650.000	350.0
Sf22T, ksi	486.000	500.000	500.000	350.0
Sf22C, ksi	486.000	500.000	650.000	350.0
Sf12S, ksi	243.000	250.000	300.000	236.0
Sf23S, ksi	243.000	250.000	300.000	236.0

^aReference 9.

^bReference 8.

^cReference 10.

^dReference 6.

TABLE II. - MATRIX PROPERTIES FROM METCAN DATABANK

Property	Matrix code name				
	TiAl ^a	Ti52 ^b	Ti6A ^c	Copr ^d	Carb ^e
Rhom, lb/in. ³	0.170	0.172	0.170	0.32	0.172
Em, Mpsi	11.600	14.700	16.500	17.7	2.5
Num, in./in.	0.260	0.350	0.300	0.3	0.22
Alfam, ppm/°F	5.000	5.000	5.240	9.8	2.12
Km, Btu/hr/in./°F	0.347	0.390	0.390	19.3	0.39
Cm, Btu/lb	0.100	0.120	0.120	0.09	0.12
SmT, ksi	65.000	144.000	144.000	15.0	10.0
SmC, ksi	65.000	144.000	144.000	15.0	10.0
SmS, ksi	52.000	90.000	90.000	9.0	10.0
EpsmT, percent	2.000	12.000	2.000	35.0	12.0
EpsmC, percent	3.000	12.000	2.000	35.0	12.0
EpsmS, percent	3.000	12.000	2.000	35.0	12.0
EpsmTOR, percent	3.000	12.000	2.000	35.0	12.0
Kvoid, Btu/hr/in./°F	0.019	0.019	0.019	0.019	0.19
Tempmm, °F	2730.000	3000.000	3000.000	1980.0	3000.0

^aReference 9.^bReference 8.^cReference 10.^dReference 6.^eLerch, Brad. Structures Division, Lewis Research Center: SCS6 Private discussions.

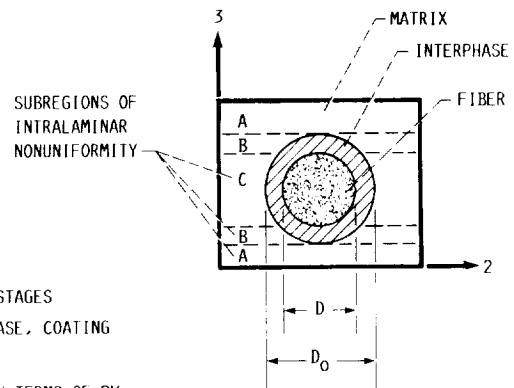
TABLE III. - TEST MATRIX FOR CHARACTERIZATION OF METAL MATRIX COMPOSITE

Test type	Properties determined	Variables						Number of tests
		T	σ	ϵ	N _M	N _T	t	
Physical/thermal	α , η , C, V _f , π	X	X				X	90
Microscopy	Interphase (R)	X	X				X	27
Monotonic UD ^a	E, ν , G, F, ϵ^u	X		X				135
Fractographic	Fracture morphology	X		X				45
Tension-compression	Monoresidual stresses							6
Cyclic (mechanical, thermal)	N _M , N _T , E, R		X		X	X		36
Monotonic MD ^b	E, ν , F, ϵ^u	X		X				81
Thermal MD ^b	α , η , C	X	X				X	81
Combined loading	E, F, ϵ^u	X						75
Loading/temp/time	E, α , η , C	X	X				X	135
Total								711

^aUD = unidirectional.^bMD = multidirectional.

$$\frac{P}{P_0} = \left[\frac{T_F - T}{T_F - T_0} \right]^n \left[\frac{S_F - \sigma}{S_F - \sigma_0} \right]^m \left[\frac{\dot{S}_F - \dot{\sigma}_0}{\dot{S}_F - \dot{\sigma}_0} \right]^l \left[\frac{\dot{T}_F - \dot{T}_0}{\dot{T}_F - \dot{T}_0} \right]^k \left[\frac{R_F - R}{R_F - R_0} \right]^p \dots$$

$$\dots \left[\frac{N_{MF} - N_M}{N_{MF} - N_{M0}} \right]^q \left[\frac{N_{TF} - N_T}{N_{TF} - N_{T0}} \right]^r \left[\frac{t_F - t}{t_F - t_0} \right]^s \dots$$



RATIONALE:

- GRADUAL EFFECTS DURING MOST RANGE, RAPIDLY DEGRADING NEAR FINAL STAGES
- REPRESENTATIVE OF THE IN SITU BEHAVIOR FOR FIBER, MATRIX, INTERPHASE, COATING
- INTRODUCTION OF PRIMITIVE VARIABLES (PV)
- CONSISTENT IN SITU REPRESENTATION OF ALL CONSTITUENT PROPERTIES IN TERMS OF PV
- ROOM TEMPERATURE VALUES FOR REFERENCE PROPERTIES
- CONTINUOUS INTERPHASE GROWTH
- SIMULTANEOUS INTERACTION OF ALL PRIMITIVE VARIABLES
- ADAPTABILITY TO NEW MATERIALS
- AMENABLE TO VERIFICATION INCLUSIVE OF ALL PROPERTIES
- READILY ADAPTABLE TO INCREMENTAL COMPUTATIONAL SIMULATION

NOTATIONS:

P - PROPERTY; T - TEMPERATURE; S - STRENGTH; R - METALLURGICAL REACTION; N - NUMBER OF CYCLES; t - TIME;
 OVER DOT - RATE; SUBSCRIPTS; 0 - REFERENCE; F - FINAL; M - MECHANICAL; T - THERMAL

FIGURE 3. - ASSUMED MULTIFACTOR INTERACTION RELATIONSHIP TO REPRESENT THE VARIOUS FACTORS WHICH INFLUENCE IN SITU CONSTITUENT MATERIALS BEHAVIOR.

- STEP I PROCESSING - COOL DOWN FROM T_p TO RT
- STEP II APPLY LOAD CYCLE TO CALCULATE σ_u AND σ_1
- STEP III APPLY THE NUMBER OF THERMAL/MECHANICAL CYCLES AND MECHANICAL LOADING INCREMENTALLY TO COMPLETE FAILURE
- STEP IV PROCESS THE OUTPUT TO OBTAIN STRESS VERSUS STRAIN DATA

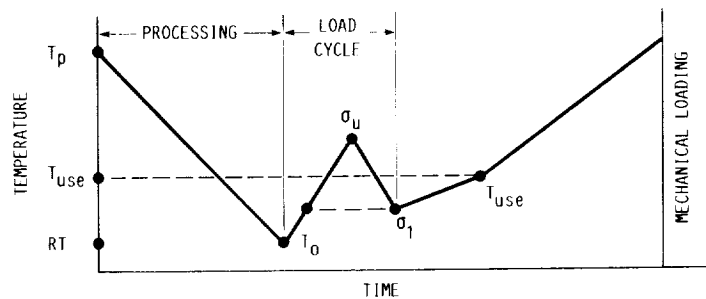


FIGURE 4. - COMPUTATIONAL PROCEDURE.

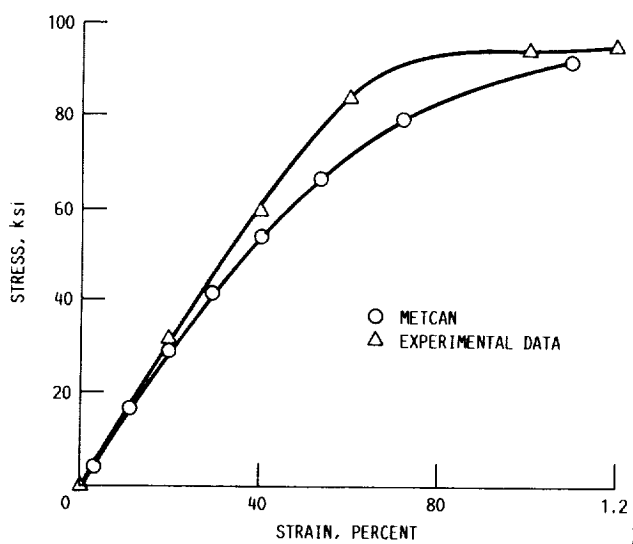


FIGURE 5. - W/Cu COMPOSITE BEHAVIOR (FVR = .280): METCAN VERSUS EXPERIMENTS.

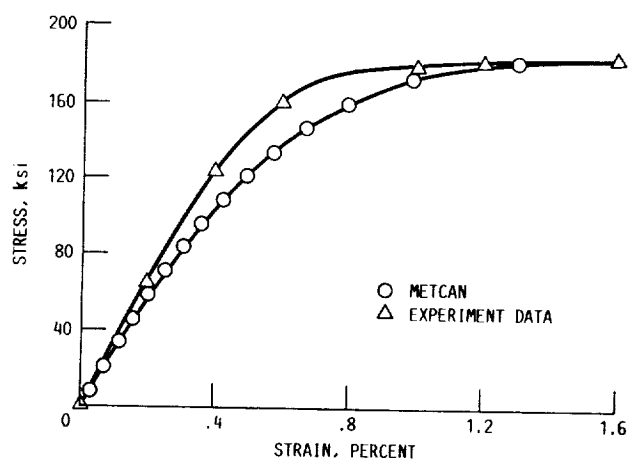


FIGURE 6. - W/Cu COMPOSITE BEHAVIOR (FVR = .536): METCAN VERSUS EXPERIMENTS.

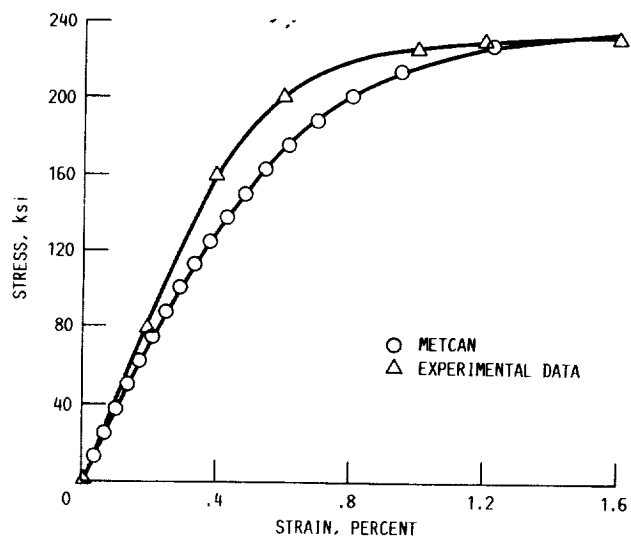


FIGURE 7. - W/Cu COMPOSITE BEHAVIOR (FVR = .674): METCAN VERSUS EXPERIMENTS.

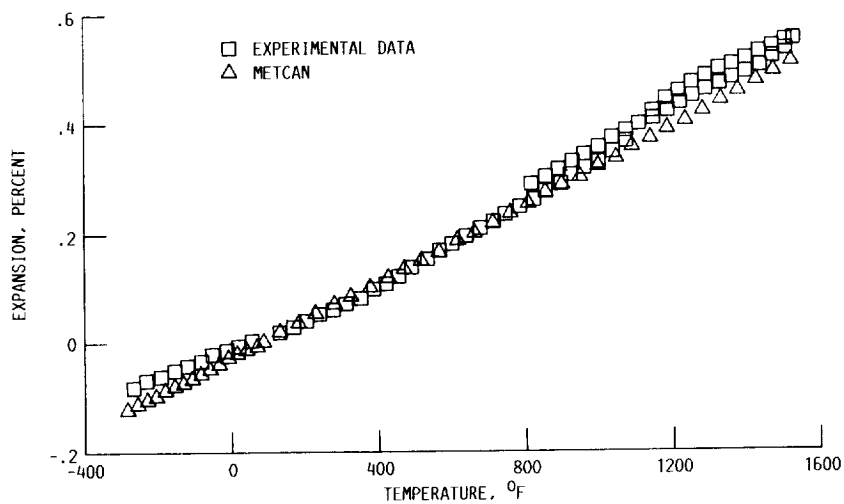


FIGURE 8. - LONGITUDINAL THERMAL EXPANSION OF [0/90/0] SiC/Ti LAMINATE AS A FUNCTION OF TEMPERATURE: EXPERIMENTAL DATA VERSUS METCAN PREDICTIONS.

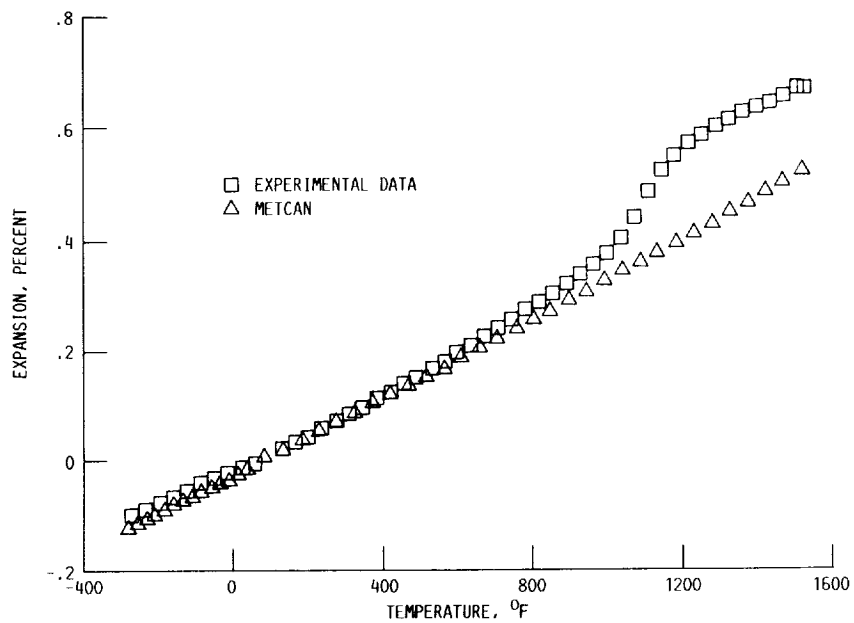


FIGURE 9. - TRANSVERSE THERMAL EXPANSION OF [0/90/0] SiC/Ti LAMINATE AS A FUNCTION OF TEMPERATURE: EXPERIMENTAL DATA VERSUS METCAN PREDICTIONS.

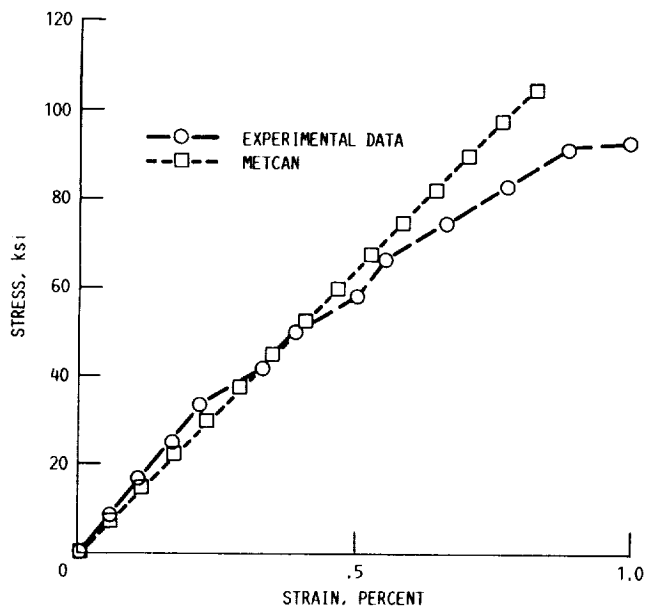


FIGURE 10. - STRESS STRAIN CURVE FOR Ti-15 MATRIX ONLY AT $T = 1022^{\circ}\text{F}$.

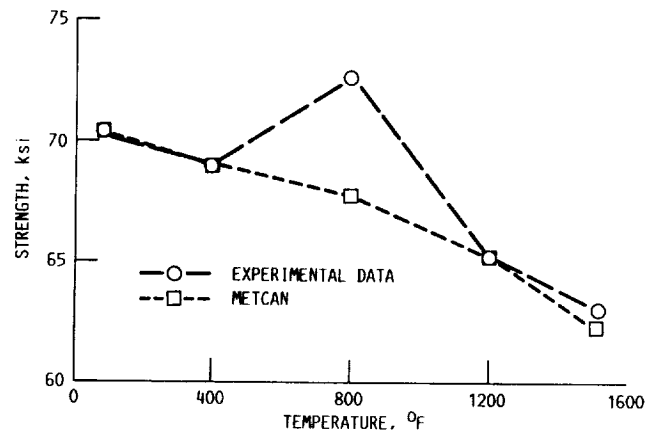


FIGURE 11. - TENSILE STRENGTH OF Ti-3Al MATRIX ONLY.

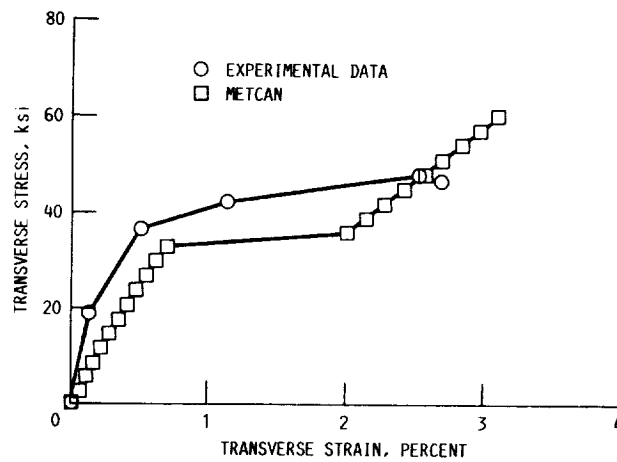


FIGURE 12. - TRANSVERSE STRESS STRAIN OF SCS 6/Ti-6-4 (FVR = 0.34, $T = 600^{\circ}\text{F}$).

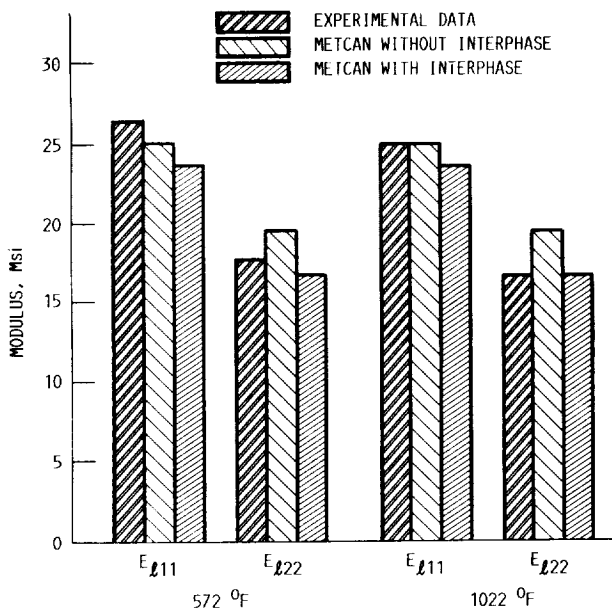


FIGURE 13. - METCAN PREDICTIONS OF MODULI FOR UNIDIRECTIONAL SCS 6/TI15 COMPOSITE (FVR = .33). (E_{11} - LONGITUDINAL; E_{22} - TRANSVERSE).

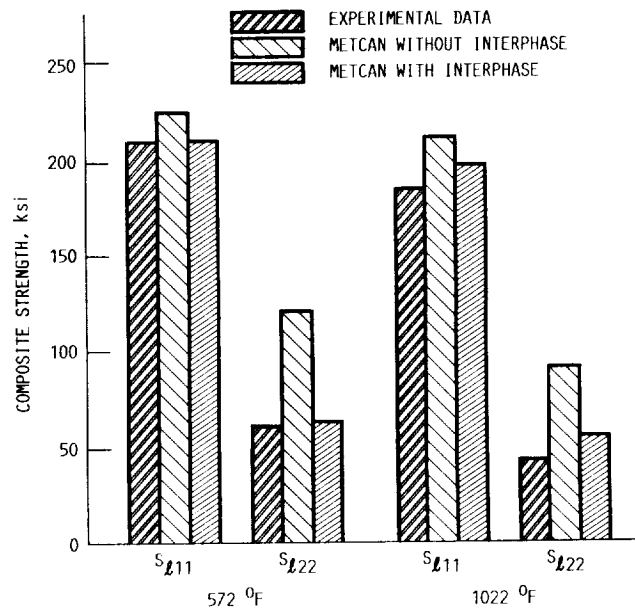


FIGURE 14. - METCAN PREDICTIONS OF STRENGTHS FOR UNIDIRECTIONAL SCS 6/TI15 (FVR = .33). (S_{11} - LONGITUDINAL TENSION; S_{22} - TRANSVERSE TENSION).

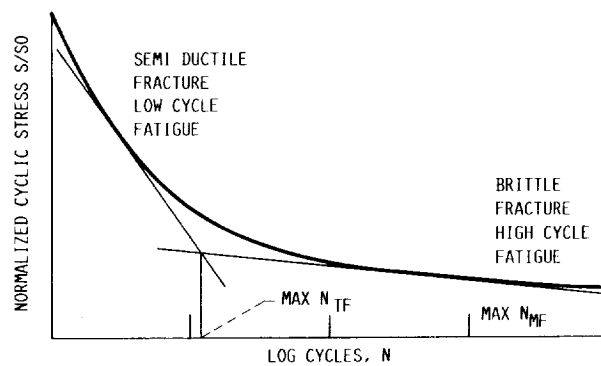


FIGURE 15. - DETERMINATION OF IN SITU MATRIX THERMOMECHANICAL CYCLIC BEHAVIOR.

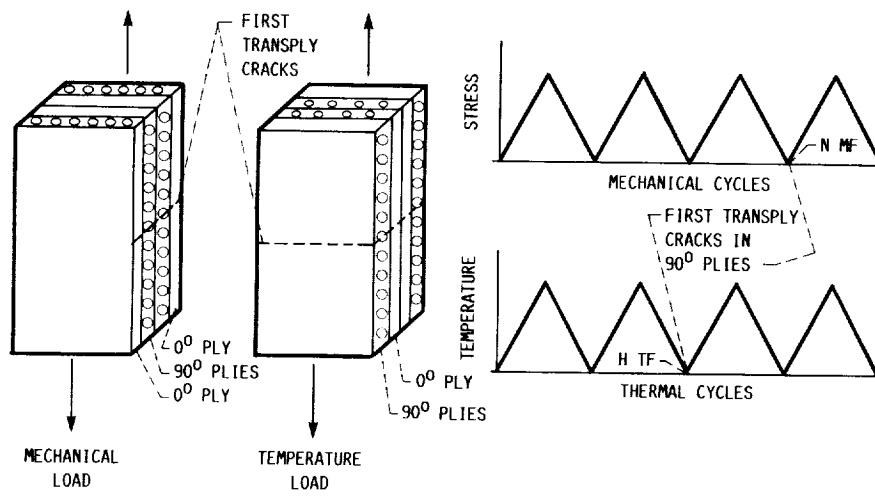


FIGURE 16. - DETERMINATION OF IN SITU MECHANICAL AND THERMAL CYCLES TO INITIATE MATRIX CRACKING.

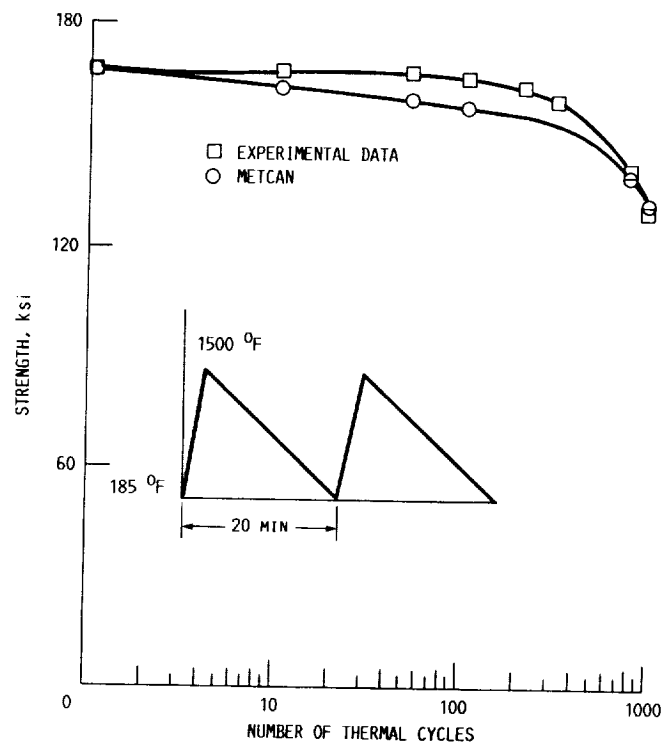


FIGURE 17. - METCAN SIMULATES THERMAL FATIGUE EFFECTS ON ROOM TEMPERATURE STRENGTH OF UNIDIRECTIONAL SiC/Ti COMPOSITE (FVR .35).

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